

O 56: Poster Wednesday: Nanostructures 2

Time: Wednesday 18:00–20:00

Location: P4

O 56.1 Wed 18:00 P4

Pt Wedge on h-BN/Rh(111): Structural Analysis by HR-XPS — •NATALIE J. WALESKA, FABIAN DÜLL, FLORIAN SPÄTH, UDO BAUER, PHILIPP BACHMANN, JOHANN STEINHÄUER, and CHRISTIAN PAPP — Friedrich-Alexander-Universität, Erlangen, Germany

An approach to overcome the material gap to commercial catalysts is the investigation of metal nanoclusters on 2D materials (e.g. h-BN). To date, mostly 3D metal clusters with a narrow size distribution on such support materials were studied. However, the clusters' structure and thus the available adsorption sites, as well as the catalytic activity varies strongly from 3D to monolayer clusters or even single atoms.

To investigate the structural differences of clusters with varying sizes, a Pt wedge was prepared in a single preparation step on the h-BN/Rh(111) substrate, ranging from 0.21 to 0.001 ML Pt coverage. The analysis was performed using HR-XPS and CO as a probe molecule. From the data, we were able to determine the transition from monolayer to 3D cluster formation for the as-prepared Pt wedge. Upon heating to 550 K, structural changes of the Pt clusters were observed as a result of cluster ripening and sintering.

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O 56.2 Wed 18:00 P4

Charge effects on the (de-)Hydrogenation activity of Pt_n-clusters on α-SiO₂ thin films — •TOBIAS HINKE¹, ANDREW CRAMPTON¹, MARIAN RÖTZER¹, MAXIMILIAN KRAUSE¹, FLORIAN SCHWEINBERGER¹, BOKWOON YOON¹, UZI LANDMAN², and UELI HEIZ¹ — ¹Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technical University of Munich, 85748 Garching, Germany — ²School of Physics Georgia Institute of Technology, Atlanta GA, U.S.A.

Catalytic model systems facilitate the gain of fundamental insights on molecular mechanisms and enable atom-precise manipulation of catalytic processes. Besides the size-effects of clusters with less than 100 atoms, the influence of the supporting material and the substrate are of special interest when steering reactivity. The catalyst's local electron density can be altered by varying the underlying metal. A high local work function of the substrate, Mo(112), yields clusters of positive charge while a low local work function, Pt(111), results in a negative charge. This allows for specifically altering the reactivity as well as the coking stability of the catalytic system.

In order to elucidate the impact of different support materials as well as cluster size-effects the change in activity of α-SiO₂ thin-film supported Pt_n-clusters towards ethylene (de-)hydrogenation was investigated. The catalytic samples were characterized in a UHV setup with base pressures below 5 * 10⁻¹⁰ mbar through IRRAS and electron spectroscopy (XPS, MIES, UPS), while reactivity was monitored with TPD and pulsed valve experiments (*p*-MBRS).

O 56.3 Wed 18:00 P4

Design of an Enhanced Ce-Evaporator for Ce_xO_y Thin Film Synthesis — •FLORA SIEGELE, KEVIN BERTRANG, TOBIAS HINKE, and UELI HEIZ — Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technical University of Munich

In today's industry, the importance of sustainability regarding resource consumption and waste management is strongly increasing and hence, the contribution of catalysis-based processes is becoming more and more important. Substantial advances can be achieved by investigating catalytic model systems to facilitate the understanding of basic mechanisms on a molecular level. These model catalysts comprise a metal single crystal substrate with metal clusters (1-100 atoms), deposited on a metal oxide thin film (2-20 ML). Especially the Lewis acidic and basic properties of metal oxides showed promising results in terms of controlled tuning of the catalytic performance. However, the reducibility of thin film materials like CeO₂ offers an additional possibility of adjusting catalytic properties. Due to the lack of experimental results focusing on the influence of CeO₂ thin films on the reactivity and selectivity of clusters, the poster presents the implementation of an optimized CeO₂ thin film generation procedure with a home-built ribbon evaporator. With this evaporator design,

including a self-built quartz crystal microbalance, deposition rates of multiple monolayers per minute could be achieved and tracked with high accuracy. Electron emission spectroscopy (x-ray photoelectron spectroscopy and Auger electron spectroscopy) was performed to investigate the composition of the deposited film.

O 56.4 Wed 18:00 P4

CO Adsorption on PdPt Alloy Nanoparticles — •DANIEL SILVAN DOLLING^{1,2}, JAN-CHRISTIAN SCHOBER^{1,2}, MARCUS CREUTZBURG¹, HESHMAT NOEI^{1,2}, and ANDREAS STIERLE^{1,2} — ¹Universität Hamburg — ²DESY

Platinum palladium alloy nanoparticles are of high interest because of their role as catalysts for different processes, including exhaust control and methane oxidation. Catalyst behavior is determined by the shape, structure and alloy composition of the particles. To enhance catalyst efficiency, it is thus necessary to improve our understanding of the structure of the nanoparticles and the active adsorption sites. In order to access detailed structural and morphological information, we employ the use of a model catalyst. In this work, platinum and palladium are co-deposited via molecular beam evaporation on α-Al₂O₃ (0001). The nanoparticles are grown epitaxially and have a well defined height to diameter ratio and alloy composition. By investigating the particle surface with the probe molecule CO using polarized infrared reflection absorption spectroscopy (IRRAS), we determined the surface species on top and side facets of the particles. The morphology was further identified with X-ray diffraction and X-ray reflectivity. The effect of the Pd/Pt alloy composition on the adsorption was investigated by comparing the IRRAS reflectivity. Moreover, the difference in the adsorption of CO was studied for samples annealed in hydrogen and oxygen.

O 56.5 Wed 18:00 P4

Methane activation with small Ta clusters — •KEVIN BERTRANG, TOBIAS HINKE, NIKITA LEVIN, MARTIN TSCHURL, and UELI HEIZ — Physical Chemistry, Department of Chemistry and Catalysis Research Center, Technical University of Munich

With the exhaustion of petroleum reserves, methane will become an important feedstock for the synthesis of fuels and fine chemicals. The challenge is to find an efficient way to activate the highly inert molecule under mild conditions and steer the reaction towards the formation of chemically precious products while preventing coking.

Studies of small cationic Ta-clusters in the gas phase and their oxides were found to exhibit high activity towards non-oxidative C-C-coupling of methane, yielding dehydrogenated carbohydrate species and ethane. The cluster charge was identified as a key parameter for activity. These studies are extended to their supported analogues. To replenish the cluster charge acidic (SiO₂) and reducible (CeO₂) thin metal-oxide films are employed and cluster oxygen content is tuned.

Characterization is performed by means of vibrational (IRRAS) and electron spectroscopy (XPS) and reactivity is studied via TPD and pulsed valve experiments.

[1] N. Levin et al. *J. Am. Chem. Soc.* **2020**, 142, 12, 5862-5869

O 56.6 Wed 18:00 P4

3d-Nanoparticles on Graphene: Influence of Temperature — •KAI BESOCKE, MAHBOOBEH RAVANKHAH, and MATHIAS GETZLAFF — Institut für Angewandte Physik, Heinrich-Heine-Universität Düsseldorf

With its unique properties, such as high quality crystal structure, excellent electrical conductivity and high tensile strength, graphene is a promising substrate for fabricating nanocomposites. In this context we are investigating the influence of graphene as substrate for the deposition of metallic nanoparticles and the influence of subsequent heating. In this contribution we present our results concerning the mobility and distribution of Fe_{0.5}Ni_{0.5}-Nanoparticles on graphene surfaces.

A W(110) single crystal serves as the substrate being coated with a Co thin film of about 20 ML and annealed at temperatures up to 500 °C. Surfaces prepared in such a way exhibit elongated Co-islands with a width of several hundred nm and height up to 10 nm, which

are coated with graphene subsequently. For graphene synthesis the samples are heated in a Propene atmosphere of 10^{-6} mbar for several minutes. The nanoparticles are produced by means of Ar magnetron sputtering in a Haberland source and aggregation takes place in a He

atmosphere. The spherical particles under investigation have diameters of several nm. Particle distributions are analyzed via STM, both as-prepared as well as after heating. It will be discussed, whether the nanoparticles are more mobile on graphene compared to other surfaces.